



IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicants: Robert B. Von Dreele

Docket No.: S-94,792

Serial No.: 09/871,527

Examiner: Carolyn L. Smith

Filed : May 31, 2001

Art Unit: 1631

For : HIGH THROUGHPUT SCREENING OF LIGAND  
BINDING TO MACROMOLECULES USING HIGH  
RESOLUTION POWDER DIFFRACTION

Commissioner for Patents  
P. O. Box 1450  
Alexandria, VA 22313-1450

**INFORMATION DISCLOSURE STATEMENT**  
**UNDER 37 CFR 1.56, 1.97, AND 1.98**

Sir:

The documents listed below are identified in compliance with the duty of disclosure defined in 37 CFR 1.56. Copies are attached as appropriate.

1. David Weininger, "Method and Apparatus for Designing Molecules with Desired Properties By Evolving Successive Populations," U. S. Patent 5,434,796, issued July 18, 1995.

**CERTIFICATE OF MAILING/TRANSMISSION (37 CFR 1.8(a))**

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Date

April 25, 2005

Signature

Bruce H. Cottrell

Bruce H. Cottrell

(type or print name of person certifying)

04/29/2005 HBLAND 00000012 122150 09871527

02 FC:1806 180.00 DA

2. Louis Crocker et al., "Polymorphic Form of a Tachykinin Receptor Antagonist," U. S. Patent 6,229,010, issued May 8, 2001.
3. Keith P. Wilson et al., "Molecules Comprising An IMPDH-Like Binding Pocket and Encoded Data Storage Medium Capable of Graphically Displaying Them," U. S. Patent 6,128,582, issued October 3, 2000.
4. Bruce Tidor et al., "Computer System and Process for Identifying a Charge Distribution Which Minimizes Electrostatic Contribution to Binding at Binding Between a Ligand and a Molecule in a Solvent and Uses Thereof," U. S. Patent 6,230,102, issued May 8, 2001.
5. Vasulinga Ravikumar et al., "Synthesis of Oligonucleotides," U. S. Patent 5,571,902, issued November 5, 1996.
6. Yen-Ho Chu et al., "Affinity Capillary Electrophoresis—Mass Spectrometry For Screening Combinatorial Libraries," J. Chem. Soc., vol. 118, pp. 7827-7835, 1996.
7. Robert Karlsson et al., "Kinetic Analysis of Monoclonal Antibody-Antigen Interactions with a New Biosensor Based Analytical System," Journal of Immunological Methods, vol. 145, pp. 229-240, 1991.
8. Shintaro Kumazawa et al., "Meed: A Program Package for Electron-Density-Distribution Calculation By the Maximum-Entropy Method," J. Appl. Cryst., vol. 26, pp. 453-457, 1993.
9. G. A. Sim, "A Note On the Heavy-Atom Method," Acta. Cryst., vol. 13, pp. 511-512, 1960.
10. Sidney Udenfriend et al., "Scintillation Proximity Assay: A Sensitive and Continuous Isotopic Method for Monitoring Ligand/Receptor and Antigen/Antibody Interactions," Analytical Biochemistry, vol. 161, pp. 494-500, 1987.
11. R. B. Von Dreele, "Combined Rietveld and Stereochemical Restraint Refinement of a Protein Crystal Structure," J. Appl. Cryst., vol. 32, pp. 1084-1089, 1999.
12. Jan Drenth, "Principles of Protein X-Ray Crystallography," Chapter 2, pp. 22-47, Springer Advanced Texts in Chemistry, 1999.
13. Allen C. Larson et al., "General Structure Analysis System (GSAS)," Los Alamos National Laboratory Report, LAUR 86-748, pp. 1-224, 2001.

14. Rex A. Palmer, "X-Ray Crystallographic Studies of Protein-Ligand Interactions," Chapter 1, pp. 1-98, 2001.
15. Romano T. Kroemer, "Molecular Modeling," Chapter 2, pp. 99-121, 2001.
16. G. N. Ramachandran, "Fourier Methods in Crystallography, pp. 1-33, John Wiley & Sons, Inc., New York, 1970.
17. Bryan John Smith, "Protein Sequencing Protocols," pp. 17-24, Humana Press, Totowa, New Jersey, 1997.
18. Anthony W. Czarnik, "Accounts of Chemical Research," Acc. Chem. Res., vol. 29, no. 2, pp. 112-113, 1996.
19. Linda C. Hsieh-Wilson et al., "Lessons From the Immune System: From Catalysis to Materials Science," Acc. Chem. Res., vol. 29, no. 3, pp. 164-170, 1996.
20. Sheila Hobbs DeWitt et al., "Combinatorial Organic Synthesis Using Parke-Davis's Diversomer Method," Acc. Chem. Res, vol. 29, no. 3, pp. 114-122, 1996.
21. Robert W. Armstrong et al., "Multiple-Component Condensation Strategies for Combinatorial Library Synthesis," Acc. Chem. Res., vol. 29, no. 3, pp. 123-131, 1996.
22. Jonathan A. Ellman, "Design, Synthesis and Evaluation of Small-Molecule Libraries," Acc. Chem. Res., vol. 29, no. 3, pp. 132-143, 1996.
23. E. M. Gordon et al., "Strategy and Tactics in Combinatorial Organic Synthesis. Applications to Drug Discovery," Acc. Chem. Res., vol. 29, no. 3, pp. 144-154, 1996.
24. W. Clark Still, "Discovery of Sequence-Selective Peptide Binding by Synthetic Receptors Using Encoded Combinatorial Libraries," Acc. Chem. Res., vol. 29, no. 3, pp. 155-163, 1996.
25. Hideo Toraya, "Position-Constrained and Unconstrained Powder-Pattern-Decomposition Methods," The Rietvelds Method, Chapter 12, pp. 255-275, International Union of Crystallography, Oxford University Press, 1993.
26. R. B. Von Dreele, "Neutron Powder Diffraction," Modern Powder Diffraction, Reviews in Mineralogy, vol. 20, Chapter 11, pp. 331-349, 1989.
27. John W. Erickson et al., "Macromolecular X-Ray Crystallography and NMR As Tools for Structure-Based Drug Design," Annual Reports in Medicinal Chemistry, vol. 27, pp. 271-289, 1992.

28. Martin R. Jefson, "Applications of NMR Spectroscopy to Protein Structure Determination," Annual Reports in Medicinal Chemistry, vol. 23, pp. 275-283, 1988.
29. U. Jonsson et al., "Real-Time Biospecific Interaction Analysis Using Surface Plasmon Resonance and a Sensor Chip Technology," Biotechniques, vol. 11, no. 5, pp. 620-626, 1991.
30. R. B. Von Dreele, "Protein-Drug Interaction," Modern Drug Discovery, vol. 4, no. 5, pp. 83-84, May 2001.
31. R. B. Von Dreele, "Combined Rietveld- and Stereochemical-Refinement with High-Resolution Powder Diffraction Data Offers a New Approach for Obtaining Protein Drug Structures," <http://lansce.lanl.gov/research/pdf/Reitveld.pdf>, pp. 1 & 2.
32. Melinda Balbirnie et al., "An Amyloid-Forming Peptide From the Yeast Prion Sup35 Reveals a Dehydrated  $\beta$ -Sheet Structure for Amyloid," Proc. Nat. Sci., vol. 98, no. 5, pp. 2375-2380, February 27, 2001.
33. J. D. Bernal et al., "X-Ray and Crystallographic Studies of Plant Virus Preparations. III," Journal of General Physiology, vol. 25, pp. 147-165, 1941.
34. W. F. van Gunsteren et al., "Biomolecular Simulation: The Gromos96 Manual and User Guide," Biomos b.v., Zurich, Groningen, pp. 1-123, 1996.
35. Xinjian Yan et al., "Ricin Inhibitors and Methods for Use Thereof," U. S. Patent 6,177,280, issued January 23, 2001.

This Information Disclosure Statement is not to be construed as a representation that a search has been made or that additional matter material to the examination of this application does not exist. Applicant does not believe that any of these citations constitutes prior art under 35 U.S.C. 102.

It is requested that the above citations be made of record in the prosecution of this application.

Respectfully submitted,

Date: April 25, 1985

Reg. No. 30,620  
Phone (505) 667-9168

Bruce H. Cottrell  
Signature of Attorney

Bruce H. Cottrell  
Los Alamos National Laboratory  
LC/IP, MS A187  
Los Alamos, New Mexico 87545

PTO form 142

## INFORMATION DISCLOSURE STATEMENT BY APPLICANT

(use as many sheets as necessary)

*Complete if Known*

Application Number	09/871,527
Filing Date	5/31/2001
First Named Inventor	Robert B. Von Dreele
Art Unit	1631
Examiner Name	Carolyn L. Smith
Attorney Docket Number	S-94,792

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Examiner Initials	Cite No.	Foreign Patent Document Country Code <sup>3</sup> - Number <sup>4</sup> - Kind Code <sup>5</sup> (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	T <sup>6</sup>
Examiner Signature				Date Considered		

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<sup>3</sup>Enter Office that issued the document, by the two-letter code (WIPO Standard ST.3)

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Substitute for form 1449B/PTO		<b>INFORMATION DISCLOSURE STATEMENT BY APPLICANT</b>  (use as many sheets as necessary)		<i>Complete if Known</i> Application Number 09/871,527 Filing Date 5/31/2001 First Named Inventor Robert B. Von Dreele Art Unit 1631 Examiner Name Carolyn L. Smith	
Sheet	2	of	4	Attorney Docket Number	S-94,792

OTHER PRIOR ART - NON PATENT LITERATURE DOCUMENTS				
Examiner Initials	Cite No. <sup>1</sup>	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published (when known)	T <sup>2</sup>	
		Yen-Ho Chu et al., "Affinity Capillary Electrophoresis—Mass Spectrometry For Screening Combinatorial Libraries," J. Chem. Soc., vol. 118, pp. 7827-7835, 1996		
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